



Spin-polarized calculations of structural, electronic and magnetic properties of Half Heusler alloys FeVX (X=Si, Ge, Sn) using Ab-initio method

M. Atif Sattar^a, Muhammad Rashid^{b,*}, M. Raza Hashmi^a, M. Nasir Rasool^a,
Asif Mahmood^c, S.A. Ahmad^a

^a Department of Physics Simulation Lab, The Islamia University of Bahawalpur, 63100, Pakistan

^b Department of Physics, COMSATS Institute of Information Technology, 44000 Islamabad, Pakistan

^c College of Engineering, Chemical Engineering Department, King Saud University, Riyadh, Saudi Arabia

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ABSTRACT

In this study, density functional theory based ab-initio calculations are utilized to investigate the electronic and magnetic properties of new series of Half Heusler FeVX (where X=Si, Ge, Sn) compounds. We have considered the $C1_b$ -type structure of these materials in three atomic configurations, termed as α , β , and γ phases, in order to find the most stable geometric structure. The structural properties of all three phases have been determined and the effect of spin-polarization has been studied. Our calculated electronic properties suggest that the studied materials under study are half-metallic (HM) ferromagnets and stable in the α -phase. We have also employed the modified Becke–Johnson (mBJ) local spin density approximation functional for a better description of the HM response of FeVX materials. We have also shown that the HM nature of FeVX compounds is robust for a wide range of lattice constant, making these materials suitable for spintronic applications.

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1. Introduction

In recent years, half-metallic (HM) materials have been a focus of considerable attention from both academic as well as industrial point of view. The interest in these materials stems from the fact that these materials are capable of showing complete spin polarization at the Fermi level (E_F) [1–3]. In the HM ferromagnetic materials, there is totally dissimilar behavior in the two spin bands. In one spin orientation, these materials display a metallic character while the other spin orientation shows a semi-conductive nature that lead to 100% spin polarization at E_F [4]. HM materials have attracted many technologists in the past decade owing to their versatile electronic property which may lead to potential applications in the spintronic devices such as nonvolatile magnetic random access memories (MRAM) and magnetic sensors [1–3], spin LED [5], spin FET [6], spin-tunneling devices [7,8].

Since the earliest of theoretical studies carried out by de Groot et al. [9] numerous HM compounds have been forecasted by different research groups [10]. To-date, HM nature has been explored

in dozens of materials such as dilute magnetic semiconductors [11–13], binary transition metal pnictides [14], chalcogenides with zinc-blende structure [15], Full Heusler (FH) compounds [16–23] and half-Heusler (HH) alloys [24–31]. The HH alloys have particularly attracted many researchers and material scientist to predict HM nature in various materials due to their high Curie temperature, structural resemblance to the zinc-blende phase, magnetic behavior and other diverse properties. Although lot of Heusler compounds have been theoretically anticipated to have HM attributes, however, the FeVX (X=Si, Ge, Sn) compounds have not received much attention both theoretically and experimentally.

In the present study, the structural, electronic and magnetic properties of FeVX (X=Si, Ge, Sn) HH compounds with $C1_b$ -type structure are investigated for the first time by performing Perdew–Burke–Ernzerhof generalized gradient approximation (PBE–GGA) [32], while the electronic properties are probed using both GGA and the modified Becke–Johnson local density approximation functional (mBJ) calculations [33]. As the GGA functional is known for underestimation of the band gap, we have utilized mBJ functional which has previously been shown to predict correct properties of magnetic materials. For instance, GGA calculations of MnAs zinc-blende predict it to be non-HM [34], whereas experimental studies [35,36] shows that it is a truly HM compound which can be confirmed by mBJ calculations [29]. Although numerous approaches

* Corresponding author.

E-mail addresses: rapakistana@yahoo.com,
muhammad.rashid@comsats.edu.pk (M. Rashid).

are available in Density Functional theory (DFT), which lead to the correct interpretation of the electronic properties, however, the simple form and cheaper computational cost makes mBJ functional ideal for studying HM materials [37–42].

2. Computational details

The structural optimization and the electronic calculations are performed by using the self-consistent full potential linearized augmented plane wave (FPLAPW) method. FPLAPW is employed into the WIEN2K code [43] based on density functional theory (DFT). For the exchange-correlation function we have used the PBE-GGA [32,44]. In this technique, the space is considered to be consisting of muffin-tin (MT) spheres, which are non-overlapping and an interstitial region between these spheres. To separate the valence and core electronic states, cut-off energy is adjusted to be -6 Ry. The spherical harmonic functions and Fourier series, originate from a basis function, are employed for MT spheres and interstitial region, respectively. The cut-off parameter for the plane wave was set to $K_{\max} \times R_{\text{MT}} = 9$, where K_{\max} is the maximum modulus for the reciprocal lattice vector. For the self-consistency cycles, energy was set to 10^{-5} Ry per formula unit and by using the modified tetrahedron method [45] for the Brillion zone (BZ) integration, 72 specific number of k-points are taken in the irreducible partition of BZ (2000 k-points in the full BZ). We performed total energy calculation for with larger k-points and found negligible differences in the total energy computed using 2000 k-points. These kinds of variables assure excellent convergence for total energy.

3. Results and discussions

3.1. Crystal structure stability

Ternary HH compounds, often referred as ternary intermetallic compounds having the chemical formula XYZ with stoichiometry 1:1:1 crystallize in the face-centered cubic $C1_b$ structure with the space group $F-43m$ (No. 216) [24]. These HH compounds can be derived from the $L2_1$ structure of a FH alloy (X_2YZ) by omitting the one X element, where X is the transition metal element and Y may be either transition metal or a rare-earth metal and Z is from the main group element. Three phases α , β , and γ can be found for the XYZ HH alloys because, in the unit cell of the HH alloy, three different atomic arrangements are possible. Crystal structure of FeVGe is shown in Fig. 1, consisting of three interpenetrating, face-centered-cubic sub-lattices, which are occupied by Fe, V, and X elements.

In order to find out the lattice constant, bulk modulus and

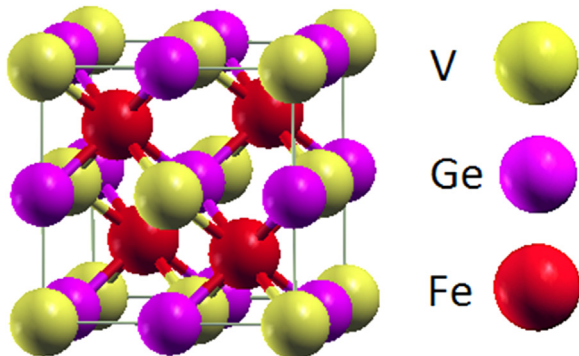


Fig. 1. Unit cell of cubic $C1_b$ -type structure for FeVGe in α -phase.

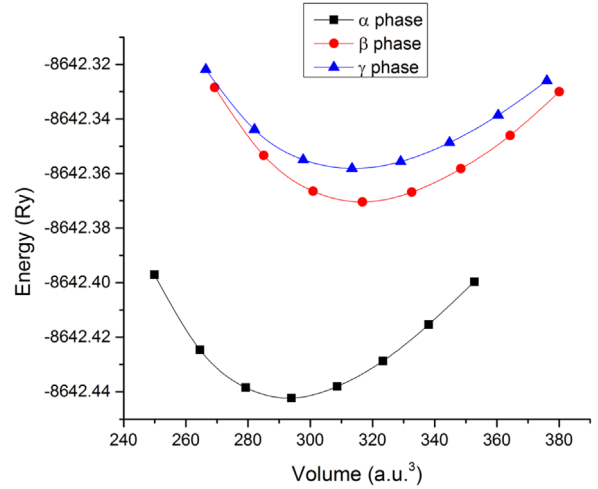


Fig. 2. Total energy as a function of volume for FeVGe in different phases (α , β , γ) of atomic positions.

Table 1

Atomic arrangement of atoms X, Y and Z in α , β and γ phases. The 4d position is actually empty.

Phase	4a (X)	4b (Y)	4c (Z)
α	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	(0, 0, 0)	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
β	(0, 0, 0)	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$
γ	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	(0, 0, 0)

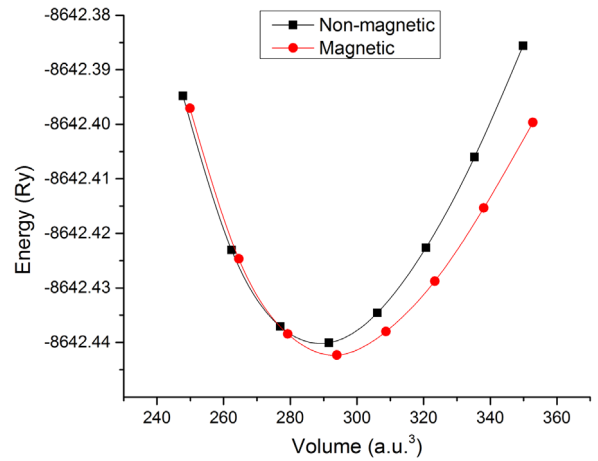


Fig. 3. Total energy as a function of volume for FeVGe in α -phase for magnetic and non-magnetic states.

energy deviations as a function of volume, geometrical optimization of HH alloys, having generic formula FeVX ($X = \text{Si, Ge, Sn}$) with $C1_b$ -type structure, have been performed by using the Murnaghan's equation of state [46]. Total energy as a function of volume is plotted in Fig. 2 for three possible phases α , β , and γ , in order to reveal the accurate atomic arrangement for primitive unit cell which is very essential because some studies show that nature of bond existing between the neighboring atoms strongly influences the physical properties [25,47]. Therefore, correct position of atoms is determined by minimizing the energy as a function of volume at their equilibrium lattice constant. The three possible phases of the FeVX ($X = \text{Si, Ge, Sn}$) HH alloy and position of these atoms for each phase (α , β , and γ) is given in Table 1. Fig. 2 shows that α -phase is more favorable than β and γ phases because it has

Table 2
Atomic optimization of the HH FeVX alloys at the α , β and γ phases, a (Å) is the lattice constant. E_{tot} and m_{tot} are the total energy and magnetic moment per formula unit respectively.

Phase	Material	Lattice constant a (Å)	Energy (Ry) E_{tot}	Magnetic moment m_{tot} (μ_B /unit cell)	Physical nature
α	FeVSi	5.46	−5024.40	1	Half-metallic
	FeVGe	5.58	−8642.48	1	
	FeVSn	5.90	−16802.51	1	
β	FeVSi	5.61	−5024.32	3.45	Metallic
	FeVGe	5.72	−8642.37	3.55	
	FeVSn	6.13	−16802.37	3.97	
γ	FeVSi	5.54	−5024.29	0.52	Metallic
	FeVGe	5.70	−8642.35	0.77	
	FeVSn	6.07	−16802.41	0.71	

Table 3
Different physical properties of HH FVX (Si, Ge, Sn) at the equilibrium lattice constant in the α -phase. V_{XC} is the exchange–correlation potential, V_{BM} is the maximum value of the valence band, and C_{BM} is the minimum value of the conduction band, E_{BG} is the energy band gap, E_{HM} is a half-metallic gap. Transition between the bands and nature of compound is also given.

Material	V_{XC}	V_{BM} (eV)	C_{BM} (eV)	E_{BG} (eV)	E_{HM} (eV)	Magnetic moment (μ_B)	Band transition	Physical state
FeVSi	GGA	0.10	0.67	0.57	–	0.92	$W \rightarrow X$	Nearly HM
	mBJ	−0.16	0.72	0.88	0.16	1.00	$W \rightarrow X$	HM
FeVGe	GGA	−0.05	0.79	0.84	0.04	1.00	$L \rightarrow X$	HM
	mBJ	−0.21	0.61	0.82	0.21	1.00	$T \rightarrow X$	HM
FeVSn	GGA	0.07	0.72	0.65	–	0.98	$T \rightarrow X$	Nearly HM
	mBJ	−0.23	0.60	0.83	0.23	1.00	$T \rightarrow X$	HM

Table 4
Total and partial magnetic moments (μ_B) of the HH FeVX (Si, Ge, Sn) compounds in the α -phase at the equilibrium lattice constant.

Compounds	Magnetic moment of individual atoms (μ_B)			Total magnetic moment (μ_B)
	Fe	V	X	
FeVSi	1.45	−0.45	0.012	1.0
FeVGe	1.84	−0.80	0.01	1.0
FeVSn	1.40	−0.41	0.011	1.0

the lowest minimized energy. These results show that the compound reside in the α -phase. To determine the magnetic ground state at the most stable structure (α -phase), both spin-polarized (magnetic) and spin-unpolarized (non-magnetic) calculations are also performed. FeVGe as a prototype, for the magnetic and non-magnetic states as a function of volume, is shown in Fig. 3, which is clearly indicating that the magnetic state has the lower energy as compared to the non-magnetic state, and therefore, is more favorable. Computed structural parameters such as equilibrium lattice constant a (Å), total energy and magnetic moment at the three different phases (α , β , γ) for the three compounds FeVX (X=Si, Ge, Sn) in the magnetic state are listed in Table 2. Moreover, the partial magnetic moments for the α -phase are arranged in Table 4.

3.2. Electronic properties

In order to explore the electronic properties of the FeVX (X=Si, Ge, Sn) at equilibrium volume, spin-polarized calculations have been studied. We will discuss electronic and magnetic properties of the FeVX HH alloys in this section and will compare the outcomes with the state-of-art mBJ-GGA results. We already know that mBJ-GGA computation only affects the electronic properties of the compounds that are underestimated or even overestimated along with GGA or LDA calculations.

We have only presented the total density of states DOS and partial DOS of the individual atoms of FeVX (X=Si, Ge, Sn) HH compounds in α -phase at the optimized lattice constant as shown

in Fig. 4. We have not shown some states such as s and p states of Fe and V because their contribution to the total DOS is very small. From Fig. 5, It can easily be visualized that total DOS is mainly contributed by the 3d states of Fe and V while p state of Ge near the E_F makes the significant contribution to the total DOS, which is also consistent with the previous HH transition-metal alloys [48,49]. The d-orbital split up into two d- e_g and d- t_{2g} orbitals. A small energy gap is found in the spin up channel due to the major contribution of d- t_{2g} orbitals of Fe and V atoms which have contributed more than d- e_g orbitals of Fe and V. The band d- t_{2g} is dominated near the fermi level. On the contrary, in the spin down channel the p orbitals of X atom crosses the E_F , leading to a metallic character for all three compounds. The most part of d-state of Fe in the spin up channel is positioned around −2.0 to −1.2 eV, whereas, in the spin down channel, this state is situated a little up around −1.8 to −0.8 eV, but d-states of V atom prevail in the energy range from −1 to 0.3 eV. The p-state of X atom is quite symmetrical in the spin up directions and crosses E_F a little in the spin down channel with a little share to the magnetism. It is also revealed from the Fig. 5, that hybridization occurs between the 3d states of Fe and V atoms. Among all the three atoms in a compound, the most part in the total magnetic moment is contributed by Fe-atom.

The different values of the physical properties of HH FeVX (Si, Ge, Sn) such as, valence band maxima (eV), conduction band minima (eV), energy band gap E_{BG} (difference between the valence band maxima to the conduction band minima) and half metallic gap E_{HM} (which is the minimum energy required to flip the electron spin across the E_F from valence band maxima), physical nature of the material and band transition calculated with both GGA and mBJ potentials, are given in Table 3. The spin up DOS has a half-metallic gap of 0.16, 0.21 and 0.02 eV for the FeVSi, FeVGe, and FeVSn, respectively, and shows the semiconducting nature. So in consequence, at the equilibrium lattice constant for the HH FeVX (X=Si, Ge, Sn) alloys in α -phase, an ideal 100% spin polarization of conducting electrons has been resulted because there appears a gap around E_F in the spin up state and at the same time DOS peak also crosses the E_F in the spin-down state.

Computed results also suggest that p-state of X-atom has the lowest part in the valance band in both majority and minority spin

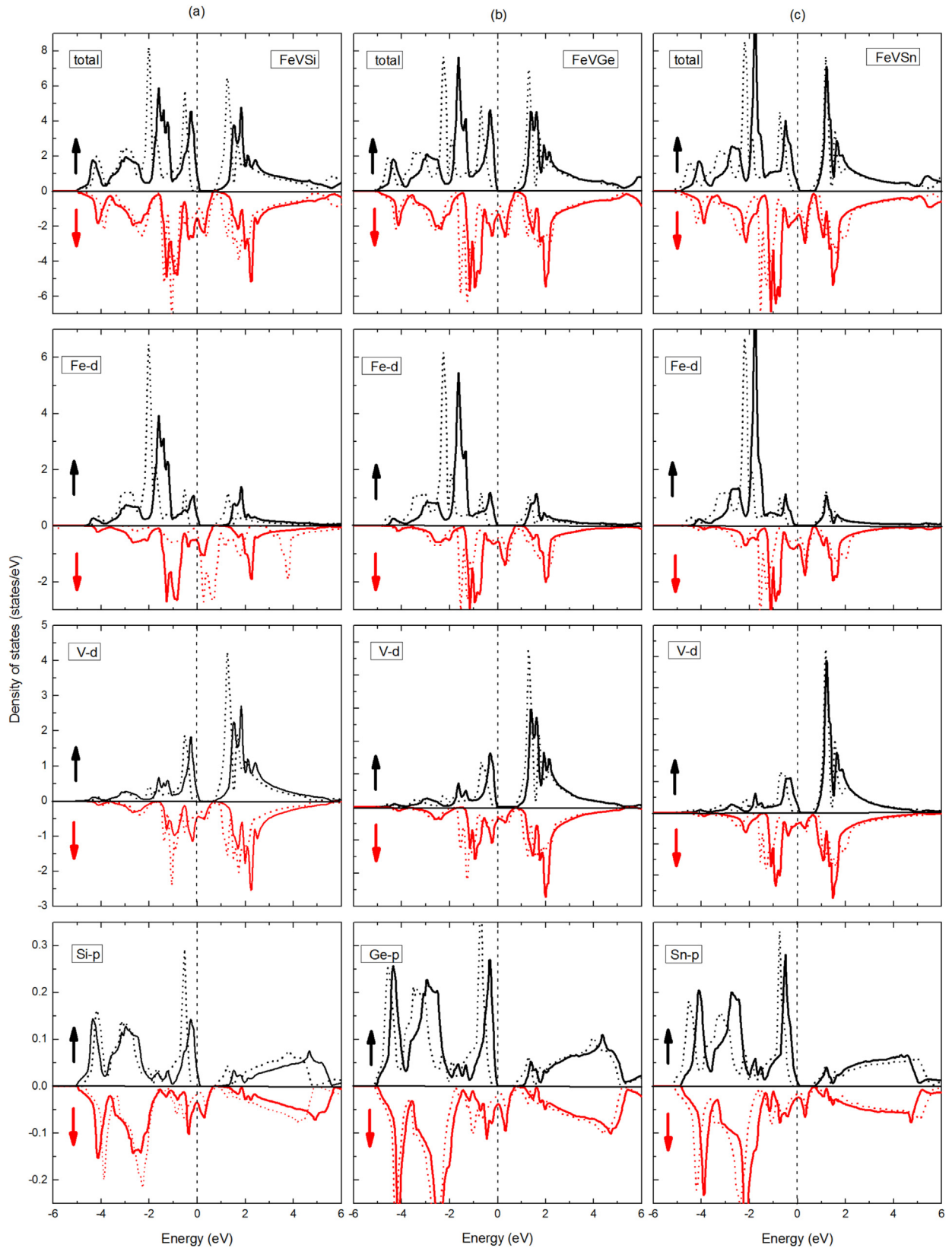


Fig. 4. Spin-dependent total and partial Density of states (DOSs) of half-metallic ferromagnetic materials (a) FeVSi (b) FeVGe (c) FeVSn at equilibrium lattice constant at the α -phase. Fermi level is set at zero. The top portion (spin-up) displays the majority-spin channel and the lower portion (spin-down) is for the minority spin channel. Solid and dotted lines show the DOS's of GGA & mBJ-GGA potential respectively.

states. In the locality of the Fermi level, d-state of Fe and p-state of X atom point out the certain dominance showing the origin of total magnetic moment will arise from Fe and X atoms. Also, the

negative magnetic moment for V represent anti-ferromagnetic alignment of the magnetic moment of V with Fe. There is large splitting in the vicinity of Fermi level due to the Fe and X-atoms

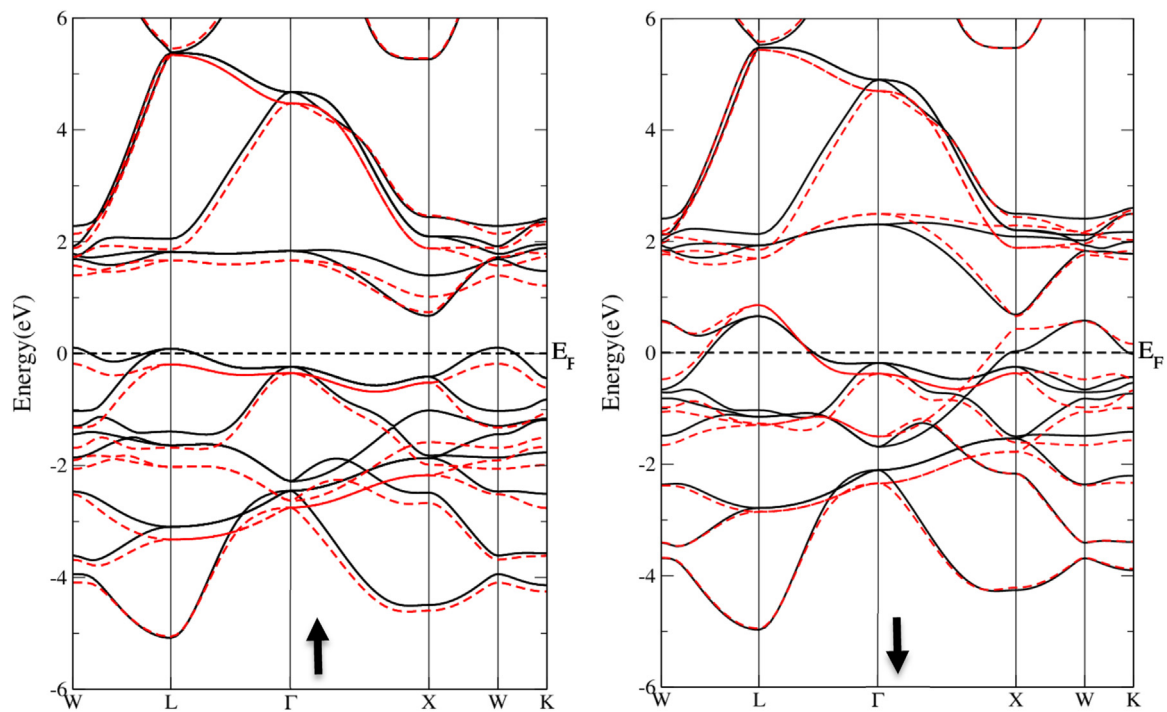


Fig. 5. Spin polarized band structure of the FeVSi for the α -phase at equilibrium lattice constant. Solid and dashed lines denote for the GGA and mBJ-GGA potential respectively.

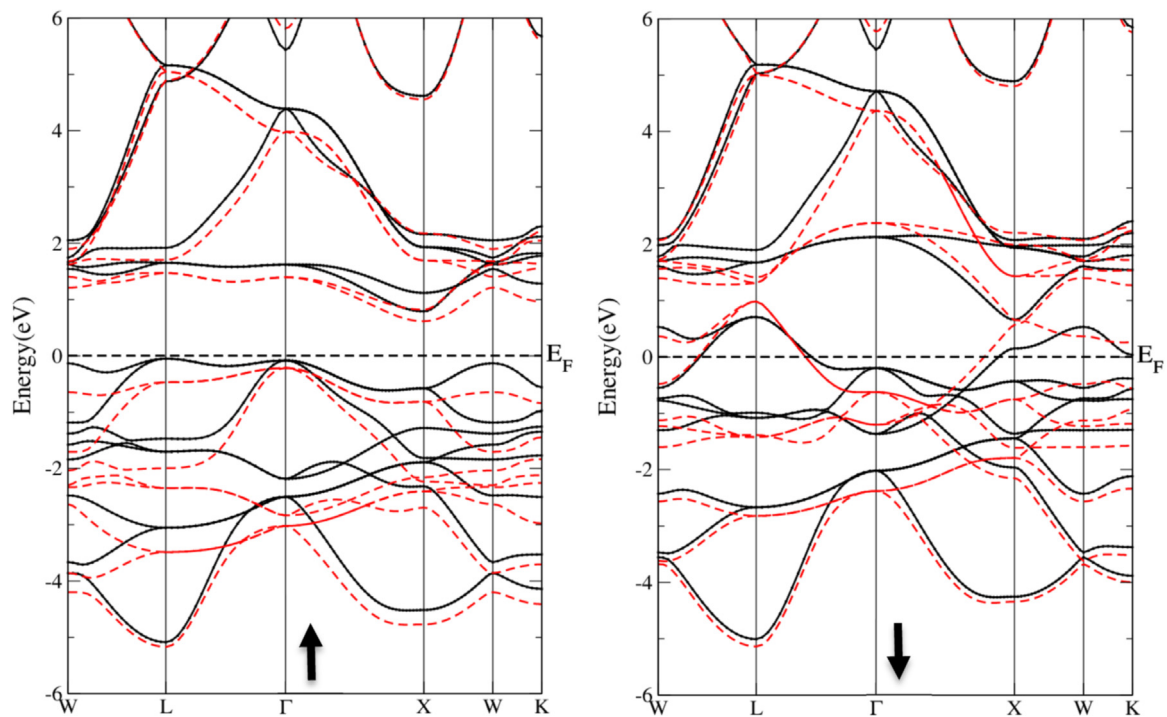


Fig. 6. Spin polarized band structure of the FeVGe for the α -phase at equilibrium lattice constant. Solid and dashed lines denote for the GGA and mBJ-GGA potential respectively.

and splitting causes the appearance of energy gap in the minority spin channel (in the spin-up state). It also reveals that Fe and X-atoms governed the energy gap in the spin up state.

Band structure calculations must be carried out very carefully because, for the prediction of HM ferromagnetism and magnetic properties of the HH compounds, electronic structure plays an important role. The band structures for all the magnetic compounds of FeVX with PBE-GGA and mBJ-GGA potentials are calculated and presented in Figs. (5–7), at their equilibrium lattice constants in the

α -phase. Left side shows the spin up (majority-spin) state and the right side shows the spin down (minority-spin) state. It can clearly be noticed that for all the FeVX compounds, the minority spin state shows no semiconducting gap and is of metallic nature, whereas the majority spin state shows the semiconducting behavior.

When GGA potential is employed to calculate band structures for the FeVGe HH compound, which shows that it is truly HM because electronic states in the minority spin channel depicting the metallic behavior, however, in the majority spin channel, there exist an energy

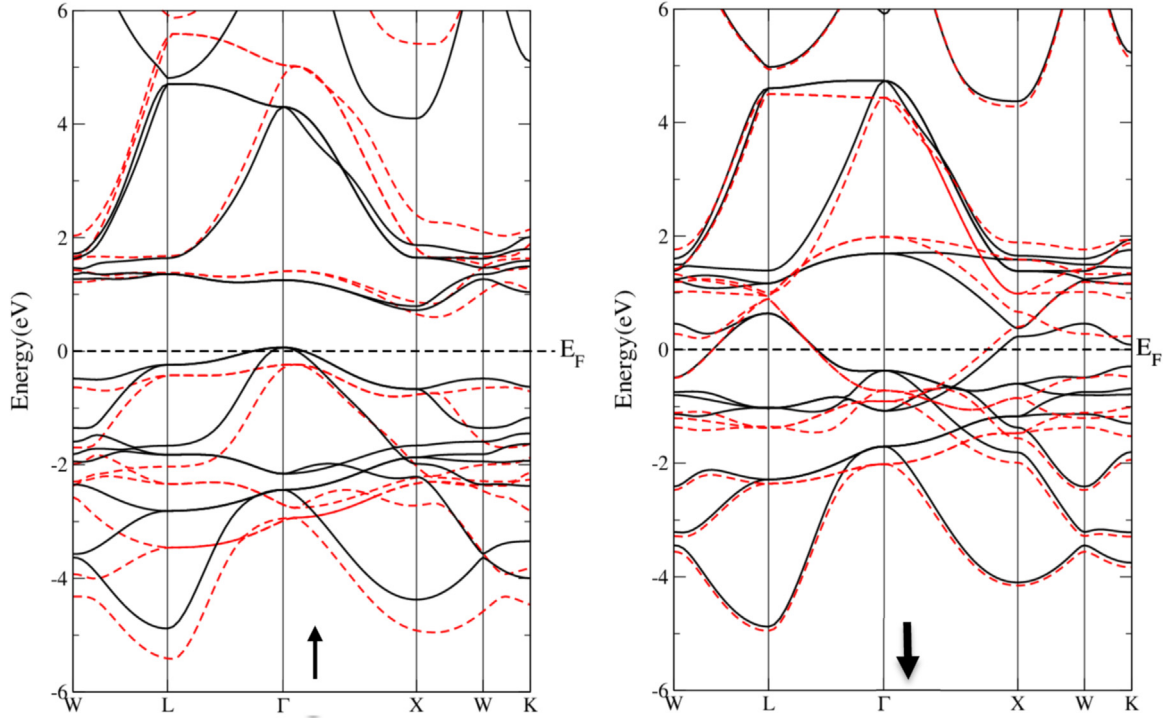


Fig. 7. Spin polarized band structure of the FeVSn for the α -phase at equilibrium lattice constant. Solid and dashed lines denote for the GGA and mBJ-GGA potential respectively.

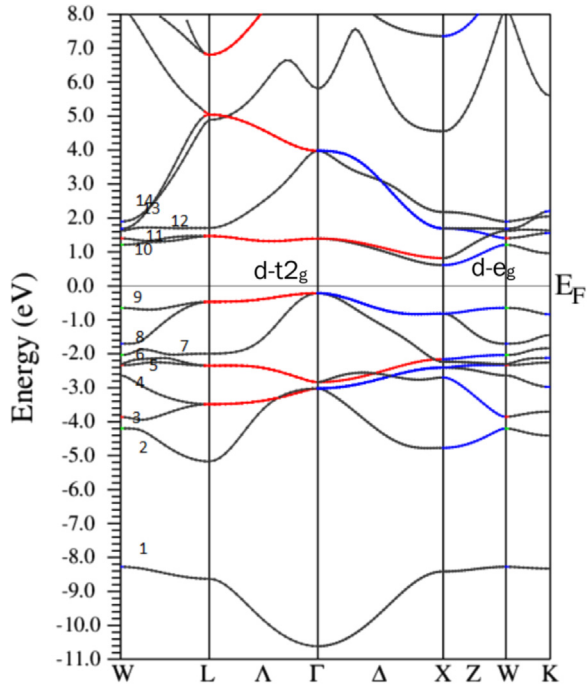


Fig. 8. Band structure of FeVGe with mBJ potential of α -phase at equilibrium lattice constant.

bandgap of 0.84 eV and electronic state do not cross E_F . The band structures of FeVSi and FeVSn compound calculated with PBE-GGA potential show that these compounds are nearly half metals because in the spin-up state very little part of the valence band crosses the E_F .

In order to improve these results obtained from PBE-GGA, mBJ-GGA potential is utilized. From PBE-GGA calculations, only FeVGe is a HM compound but when calculations are made from mBJ-GGA potential, it is observed that valence bands are now shifted

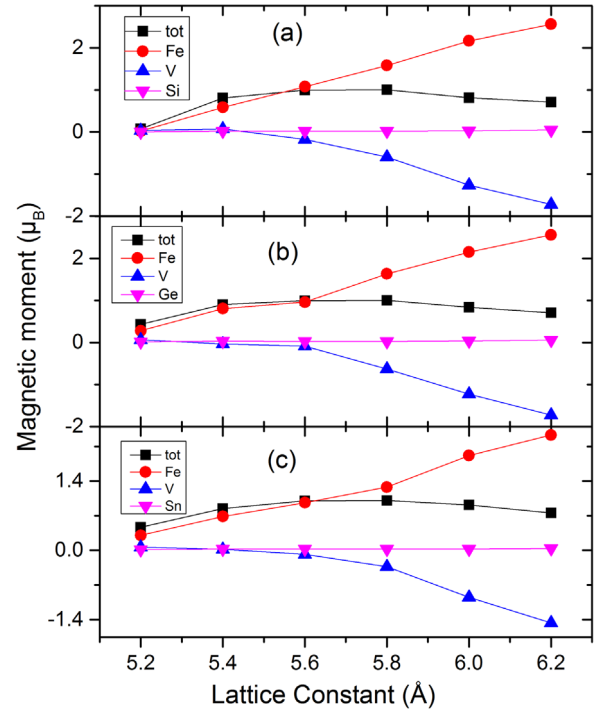


Fig. 9. Magnetic moment as a function of lattice constant (a) FeVSi, (b) FeVGe & (c) FeVSn.

downwards and conduction bands are shifted upwards for all the FeVX compounds. The values of both E_{BG} and E_{HM} are also increased and now, all these compounds are truly HM materials.

3.3. Magnetic properties

The total and partial magnetic moment m_{tot} and magnetic moment of the individual atoms (in the units of μ_B) for the HH

FeVX(Si, Ge, Sn) per formula unit cell for the α -phase are summarized in Table 4. To understand the semiconducting gap, Fig. 8 illustrates the spin-polarized band structure of FeVGe (up-state) in the α -phase at the equilibrium lattice constant. Band 1 is of the s-state of the Ge, which has the lowest part in the valance band for both majority and minority spin states. Bands 2–4 and 12–14 are because of the p-state of Ge whereas bands 3–6 are because of d-states of the Fe and 7–11 consists of d-states of V. The d-orbitals further splits up into double degenerated d- $e_g(2)$ and triplet degenerated d- $t_{2g}(3)$ states due to the crystal field effect. Bands 7–9 at Γ are because of the d- t_{2g} states of the Fe atom below E_F . Above E_F , bands 10 and 11 located at X are due to the d- e_g states of the V atom. Bonding and antibonding states are formed because these triplet d- t_{2g} states of Fe interact with the sp^3 -type states of V atom. It means that triply degenerated d- t_{2g} state of Fe and doublet degenerated d- e_g state of V in the spin up channel should be occupied as in the spin down channel, but by the exchange interaction, electrons get depleted in these occupied states and becomes unoccupied and governs the semiconducting gap.

3.4. Half-metallic robustness

HM robustness is the transition of a material from HM to pure metallic nature. Finally, for the useful applications of HH alloys in the spintronic, HM stability for the FeVSi, FeVGe, and FeVSn compounds is explored over a wide range of lattice constant. As thin films or multiple layers of HM materials are used to grow on suitable substrate for spintronic devices, therefore, lattice constant of the deposited thin films may change and this can destroy the half-metallicity of the HH materials. Hence, it is very essential to know how far lattice constant of FeVSi, FeVGe, FeVSn HH materials should be varied so that they keep their half-metallicity. Due to this reason, the relationship between the total magnetic moment and the spin magnetic moment of Fe, V, and X atoms and its reliance on the lattice parameters is shown in Fig. 9. It can be revealed that as lattice parameter of FeVX (X=Si, Ge, Sn) compounds are extended or contracted from their theoretical equilibrium lattice constant, the hybridization between the Fe and V atoms changes. For all the three compounds, when the lattice parameter is boosted, it increases the magnetic moment of the Fe and decreases the magnetic moment of the V but the total magnetic moment per unit cell changes slightly and remains approximately at $1 \mu_B$, which is integral multiple of Bohr magneton. FeVSi, FeVGe, and FeVSn retain their HM property within the lattice constant range of 5.25 Å to 5.75 Å, 5.18 Å to 5.8 Å and 5.20 Å to 5.90 Å, respectively. i. e, Fermi level remains in the gap and these alloys keep their half-metallicity when the lattice constants of FeVSi, FeVGe and FeVSn are contracted and extracted up to 3.84–5.31%, 3.91–5.91% and 3.94–11.8% respectively, from their theoretical equilibrium lattice constant.

4. Conclusion

In summary, we have performed a detailed investigation of new series of potentially HH FeVX (X=Si, Ge, Sn) compounds by employing GGA mBJ exchange-correlation energy functional of density functional theory. Our GGA results indicate that FeVGe is half metallic, while FeVSi, FeVSn are metallic. On the other hand, the mBJ calculations reveal that FeVSi, FeVGe, and FeVSn compounds are excellent HM having integer magnetic moment of $1 \mu_B$ and half-metallic gaps of 0.16 eV, 0.21 eV, and 0.23 eV respectively. We found that the ferromagnetism arises from Fe-d states along with a small contribution of p-states of X-atoms. The band-gap appearing in the spin up channel is due to strong d-d hybridization of transition metals (Fe and V). FeVSi, FeVGe, and FeVSn retain their HM when their lattice parameters are changed in the range

3.84–5.31%, 3.91–5.91% and 3.94–11.8% respectively and therefore, they could be considered as a potential candidate for the useful spintronic applications.

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